AD-786 216

THERMODYNAMICS OF COMBUSTION OF VARIOUS PYROTECHNIC COMPOSITIONS

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Prepared for:

Naval Air Systems Command

11 June 1974

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

AD-786 216

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER RDTR No. 277	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) THERMODYNAMICS OF COMBUSTION OF VARIOUS PYROTECHNIC COMPOSITIONS		5. TYPE OF REPORT & PERIOD COVERED FINAL REPORT January 1971 - July 1973 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) John E. Tanner, Jr.		8. CONTRACT OR GRANT NUMBER(s)
9. PERFORMING ORGANIZATION NAME AND ADDRESS Naval Ammunition Depot Applied Sciences Department Crane, Indiana 47522		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS AIRTASK A350-350F/159B/4F-546-503
11. CONTROLLING OFFICE NAME AND ADDRESS Commander Naval Air Systems Command (Code AIR-350E) Washington, D. C. 20360		12. REPORT DATE 11 June 1974 13. NUMBER OF PAGES 24
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Pyrotechnics, Thermochemistry, Thermodynamics, Combustion

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Heats of reaction and/or adiabatic flame temperature have been computed for a variety of compositions of interest to pyrotechnics. One set of compositions includes pairwise fuel/oxidizer combinations consisting of magnesium, aluminum, beryllium, boron, carbon and silicon with alkali oxides, alkali nitrates, alkali perchlorates, teflon, air and a few other substances.

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S/N 0102-014-6601

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It has been found that the oxidizers differ from each other in approximately the same manner, regardless of which fuel is used, and similarly, the fuels differ in the same way regardless of which oxidizer is used. Significant differences in flame temperatures and heats of reaction are noted among the alkali nitrates, in spite of their similar chemistry.

Using a perchlorate as oxidizer, a large percentage of the associated alkali metal is combined as the chloride even at the adiabatic temperature.

Of six aluminum compounds tried, aluminum carbide may be competitive with magnesium metal.

Of six sodium compounds tried, the pure metal, the hydride, and the carbide are the most promising for sodium enrichment of illuminating flares.

APPROVED BY

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SUMMARY

When new or improved pyrotechnic compositions are being designed, the basic thermodynamic properties of the components and of their combustion are of immediate interest. These properties include the adiabatic flame temperature, the heat of reaction, the optimum fuel/oxidizer ratio and the concentrations and phases of product species, especially those which emit light in a wavelength range of interest. In three separate studies, flame temperature and heats of reaction have been computed for various fuel/oxidizer combinations.

The first study was a comparison of the alkali nitrates, a few oxides of sodium, hydrogen peroxide, teflon, air and oxygen as oxidizers and a comparison of aluminum, magnesium, beryllium, boron, iron, silicon and iron as fuels. About half of all the possible fuel/oxidizer pairs were formed.

It has been found that generally the oxidizers differ from each other in approximately the same manner, regardless of which fuel is used, and similarly, the fuels differ in the same way regardless of which oxidizer is used. An exception is air, whose rank among the oxidizers varies with the fuel used. Of the fuels, boron and carbon exhibit some irregularities. Significant differences in flame temperatures and heats of reaction are noted among the alkali nitrates, in spite of their similar chemistry.

Where a perchlorate was used as an oxidizer, a large percentage of the associated alkali metal was combined as the chloride ever at the adiabatic temperature. This is a disadvantage for illumination purposes.

The purpose of the second study was to compare aluminum compounds as fuels for illuminating flare compositions. Of the six compounds computed, aluminum carbide has properties which may be competitive with those of magnesium. None of the compounds excelled or exceeded pure aluminum.

The purpose of the third study was to determine which sodium compounds are thermodynamically the most promising for enrichment of illuminating compositions. The most promising of six tried were found to be the pure metal, the carbide, and the hydride.

PREFACE

The Applied Sciences Department is funded to conduct exploratory studies aimed at the development of better pyrotechnic flares for signaling and illumination. The information presented here is a partial result of these efforts. A portion of these results have already been presented in RDTR No. 253, "Theoretical Light Yields From Different Illuminating Flare Compositions." See reference 1.

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INTRODUCTION

Numerous computations of flame temperatures and heats of reaction have been made for pyrotechnic compositions,[2,3] including a few of the compositions mentioned later in this report. In order to compare a set of compositions, the computations should all be done with the same set of thermodynamic data for the reactants and products. For this reason we have repeated the computations of such well known formulations as $Mg/NaNO_3$/binder in order to compare with other formulations for which we could find no previous computations.

For computations of flame temperatures or of heats of reaction to products at an elevated temperature, we used the NASA computer program of Gordon and McBride.[4]

This versatile program can be used in many ways. In one option used here, a set of formulas and their heats of formation are supplied, along with the specification of the relative amounts of each and of the confining pressure. The program then computes the equilibrium temperature and mole fractions of products corresponding to adiabatic conditions.

The other option used here was to specify the final temperature. In this case, the program computes the equilibrium mole fractions of products and the final total enthalpy.

Three separate studies are presented. In the first, we compared a number of common fuels and oxidizers in simple mixtures along with a common binder. In the second study, various aluminum compounds were compared as fuels for illuminating formulations. In the third study, several sodium compounds were compared as candidates for increasing the sodium content of illuminating formulations.

FUEL/OXIDIZER PAIRS

Method

A small selection of common inorganic fuels and oxidizers has been made. Thermodynamic properties have been computed for the combustion of about half of all of the possible fuel/oxidizer combinations. For all combinations involving a solid fuel and oxidizer, five percent of epoxy binder is included, of formula $C_{5.75}H_{8.36}O_{1.15}N_{0.3}$.

The first step was to find for each combination the fuel/oxidizer ratio giving the highest adiabatic equilibrium temperature. The results obtained in this step also included the species mole fractions at this temperature and the theoretical density for the initial composition.

In a subsequent computation the energy of reaction was computed for reactants initially at 298K going to products at 1200K. This latter temperature was chosen as a cutoff point, below which negligible visible radiation would be given off as the reaction products cool.

The equivalence ratios were computed by dividing the weights of fuel and oxidizer by their respective gram equivalent weights, using the following valences: the fuel its maximum valence, oxygen = 2, fluorine = 1, nitrogen, chlorine, and the alkali metals = 0. The reason for assigning zero valence to nitrogen is that it usually ends almost entirely as N_2. The alkali metals usually are in the atomic form at high flame temperatures. With the small amounts of chlorine used, the major part of it ends as a chloride of the alkali, which was already assigned zero valence. Smaller amounts do act as an oxidizer for the metal fuel and the binder. However for simplicity it was counted as inert rather than assigning to it a fractional valence, which would have been less than 0.5.

Results and Discussion

Temperatures and Heats of Reaction

The two quantities which are most important in giving an indication of the amount of energy available for visible light output are the adiabatic flame temperature (K) at equilibrium and the heat of reaction (kcal per gram of solid). These are presented together in Table 1 . They correspond to the fuel/oxidizer ratios giving the maximum adiabatic temperature. Remember that the heats of reaction are for reactants at 298K going to products at 1200K.

The optimized compositions are presented in Table 2. For each composition, the first line gives the weight percent of the fuel listed in the left hand column. The next two lines give the fuel/oxidizer equivalence ratio without, and with consideration of the binder, respectively. Since the binder is a fuel (the equivalent weight of epoxy binder is 3.44) the second number is always larger than the first.

In comparing the alkali nitrates, the small differences in adiabatic temperature are much magnified in the heats of reaction. This is partially due to the varying amounts of alkali metal oxidized at the cutoff temperature of 1200K (data not presented). A computation with products at 298K would show the various alkali nitrates to have more nearly equal heats of reaction.

In the case of silicon, comparing sodium nitrate with sodium perchlorate, a small difference in adiabatic temperature corresponds to a large difference in heat of reaction. Again it is a matter of the degree of reaction of the sodium at the cutoff point of $1200^{o}K$. At this temperature the perchlora e sodium is completely combined as chloride, whereas the nitrate sodium is mostly in elemental form, and will liberate a large amount of energy when it reacts with the water and other oxides present as the temperature is lowered toward 298K.

The high heats of reaction obtained with air or oxygen as the oxidizer are not the result of any unusual chemistry, but simply result from not including them in the calculation of the total weight of reactants. This was done because in actual usage these gases are in the environment and thus may be had "free".

Optimum Fuel/Oxidizer Ratios

Generally it can be expected that a stoichiometric mixture yields the highest temperature. However, several factors can cause this expectation not to be precisely fulfilled:

The most common deviation here is caused by the competition between two fuels of greatly different reducing powers--a metal and a binder. An optimum is reached when the weaker fuel is only partly oxidized. Hence in nearly all cases in Table 2, the optimum equivalence ratio counting the binder, and that not counting the binder lie on opposite sides of unity. The closer the latter is to unity, the more successful the metal is in excluding the binder from the available oxygen.

When the product of combustion is considerably dissociated at equilibrium, the optimum is shifted in the direction of the component having the lowest heat capacity

and/or the most positive heat of formation. This is well demonstrated in the mixtures with air, where the optimum fuel/oxidizer ratios are relatively high.

The low equivalence ratios seen in the combinations of carbon and iron with sodium nitrate can be explained by the low flame temperatures in these cases. The sodium is able to compete for the oxygen and so should have been included as a fuel in calculating the fuel/oxidizer equivalence ratio.

Reaction Products

There is a wealth of information in the listings of reaction products in Table 3. Only a few things will be pointed out:

For all but the weakest fuels, carbon and iron, the alkali elements are present mostly in the atomic form when chlorine is absent. Except for the case of lithium, the atomic form accounts for more than 95% of the total.

When perchlorate is the oxidizer, however, a large portion of the alkali elements are present in the form of the chloride. Other calculations (not presented) show that the percentage of chloride increases rapidly as the mixture cools below the adiabatic temperature.

The metals vary considerably in the extent of dissociation of the oxidation product at equilibrium. Magnesium oxide or chloride is the least stable, with increasing stability for the compounds of aluminum, beryllium, boron, and iron, in that order.

Boron nitride is sufficiently stable so that nitrogen can be an effective oxidizer of boron after all the oxygen has been consumed, and can influence the optimum composition. An example is seen in the case of boron plus air.

Table 4 gives computed densities of various fuel-oxidizer combinations.

Example of a Prediction

The purpose of accumulating this data has been to help in predicting luminous output. As an example, we might use the numbers in Tables 1 and 2 to predict relative output of the sodium-containing oxidizers used with magnesium as fuel.

The heats of reaction and adiabatic temperatures both indicate that light output when using sodium peroxide (Na_2O_2) should be much lower than for the other cases. This has been verified by experiment.

Sodium superoxide should have a slight edge over sodium nitrate due to a somewhat higher heat of reaction and a significantly higher sodium atom content.

A comparison between sodium perchlorate and sodium nitrate is more difficult. The thermodynamic factors both favor the sodium perchlorate, but the tying up of the perchlorate sodium by the chlorine operates in favor of the nitrate as yielding the greater light output. A computation where these factors are combined in a more sophisticated manner might be able to successfully predict the result.

ALUMINUM COMPOUNDS

Introduction

Aluminum has for some time been considered a very promising compound for illumination pyrotechnics because of the high flame temperatures which it is theoretically capable of attaining in combustion. Test results have not borne out these expectations. The failure is believed due to incompleteness of combustion of the aluminum, which is in turn caused by the very low volatility of the metal and its oxide.

One way of more completely exposing all of the aluminum to the oxidizer would be to have it present in the form of a molecular compound, with the other elements being more volatile. A penalty would be paid for the presence of these elements, since they would almost certainly have lower energies of combustion, and thus would lower the reaction temperature.

We have here investigated which aluminum compounds would be most promising by computing adiabatic flame temperatures of various ones, in each case reacting with a stoichiometric amount of sodium nitrate. No binder is included. Where carbon or sulfur is involved and the stoichiometry is in doubt, several fuel/oxidizer ratios were calculated and the maximum temperature estimated.

Results and Discussion

The computed flame temperatures of the aluminum compounds and of magnesium are presented in Table 5. As expected, all of the calculated adiabatic temperatures fall below that for metallic aluminum. Futhermore only one compound, aluminum carbide, gives an adiabatic temperature above that for magnesium metal, which is the present standard pyrotechnic fuel.

It is doubtful that aluminum carbide is promising even from a thermodynamic standpoint in comparison to magnesium for illumination pyrotechnics. Although the former has a higher theoretical flame temperature, this would be at least partially offset by its lower heat of combustion.

ENRICHMENT WITH SODIUM COMPOUNDS

Introduction

It is well known that the principal emitter in illumination formulations is the sodium atom. The possibility exists then that an increase in the sodium content of the composition might increase the light emission.

The final result will be determined by several conflicting factors. One of these is that sodium compounds are not very energetic in the flare reactions, and thus their presence will decrease the flame temperature.

To determine which sodium compounds would be most promising for increasing the sodium content, we have computed flame temperatures for a basic mixture of 3 moles magnesium and 1 mole sodium nitrate, to which an additional mole of sodium-containing compound is added. This additional mole is balanced between the compound under consideration and a stoichiometric amount of sodium nitrate. Thus the proportions when adding sodium amide are: $3\ Mg + 1.25\ NaNO_3 + .75\ NaNH_2$. In computing stoichiometry, several valences were tried for carbon and sulfur. Those giving the maximum temperatures were 3 and 4, respectively.

Results and Discussion

The compositions and computed adiabatic flame temperatures are presented in Table 6. It can be seen that, judging by computed flame temperature, the best method of increasing sodium content is by the addition of metallic sodium itself. Next best would be the addition of the hydride or carbide.

Although heats of reaction have not been computed for these formulations, it seems probable that they lie in about the same order as the flame temperatures.

REFERENCES

1. H. A. Webster III, J. E. Tanner, Jr., and B. E. Douda, Theoretical Light Yields from Different Illuminating Flare Compositions, RDTR No. 253, NAD Crane, Indiana (July 1973). AD#767 928.

2. S. Katz, E. Raisen, K. D. Franson, P. K. Ase, and R. Rimkus, A Study of New Materials Related to the Development of Infrared Countermeasures for Aerial Systems, Technical Report ASD-TR-62-1009, Wright-Patterson Air Force Base, Dayton, Ohio (December 1962). AD#340 230.

3. E. Raisen, P. K. Ase, B. J. Northan, and R. H. Snow, Thermochemical Investigations of Pyrotechnic Compositions, Report No. U6058-15, Illinois Institute of Technology Research, Chicago, Illinois (1968). AD# 839 545.

4. S. Gordon and B. J. McBride, Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouquet Detonations, NASA SP-273, Lewis Research Center (1971).

TABLE 1

Computed adiabatic temperatures (K) and heats of reaction (kcal/g, products at 1200K) of fuel-oxidizer combinations. 5% epoxy binder is included where both fuel and oxidizer are solids.

	$LiNO_3$	$NaNO_3$	KNO_3	$CsNO_3$	$NaClO_4$	$KClO_4$	NaO_2	Na_2O_2	H_2O_2	$-CF_2-$	Air	O_2
Al	3361 2.15	3371 1.47	3326 1.20	3146 .64	3594 2.32	3580 2.08	3460 1.65	2260 .49	3440 3.00	3460	3549 5.97	4019 6.95
Mg	3084 1.93	3073 1.45	3056 1.17	2970 .63	3156 2.08	3154 1.89	3089 1.64	2339 .56	3150 2.70	3400 1.93	3053 3.66	3347 5.48
Be		3554 1.98			3736 2.97					3607	3538 12.9	
B		2151 1.16			3151 2.03					3518 1.20	2728 7.1	
Fe		1775 2.81			2727							
Si		2855 1.10			2998 1.93						2846 5.6	
C		1640 .33			2756 .93						2236 4.4	

TABLE 2

Weight percent fuel and fuel/oxidizer equivalence ratios to produce the maximum computed adiabatic temperature.

	$LiNO_3$	$NaNO_3$	KNO_3	$CsNO_3$	$NaClO_4$	$KClO_4$	NaO_2	Na_2O_2	H_2O_2	Air	O_2
Al	38.7[a] .87[b] 1.17[c]	34.4 .90 1.24	30.3 .88 1.25	17.1 .79 1.40	34.5 .97 1.34	31.3 .94 1.34	35.2 .90 1.23	27.2 .87 1.28	50.3 .95	20.6 1.07	52.4 .98
Mg	43.0 .78 1.10	39.9 .85 1.22	35.2 .82 1.23	20.2 .72 1.36	38.1 .85 1.24	35.1	40.8 .85 1.22	33.0 .85 1.31	53.5 .80	29.0 1.24	60.2 1.00
Be		21.3 .91 1.19			20.6 .94 1.24					11.2 1.04	
B		17.6 .89 1.16			15.7 .84 1.12					22.2 2.92	
Fe		39. .53 .90			49. .89 1.37						
Si		26.8 .80 1.10			26.4 .84 1.17					17.5 1.12	
C		10.6 .60 .84			14.2 .90 1.17					7.8 1.05	

a – Weight percent fuel
b – F/O equivalence ratio not counting binder
c – F/O equivalence ratio counting binder

TABLE 3
MOLE FRACTIONS OF REACTION PRODUCTS
(A) ALUMINUM FUEL

$LINO_3$

AL	.00576
ALH	.00003
ALO	.00224
ALOH	.00052
ALOH+	.06199
ALO2	.00062
ALO2-	.02891
ALO2H	.00054
AL2O	.00123
AL2O2	.00001
AL2O3(L	.21810
CO	.10362
CO2	.00458
CO2-	.00003
E	.03279
H	.03952
H-	.00003
H2	.01116
H2O	.00385
LI	.28068
LI+	.00001
LIH	.00092
LIN	.00001
LIO	.00412
LIO-	.00002
LIOH	.01780
LI2	.00018
LI2O	.00211
N	.00004
NO	.00292
NO2-	.00001
N2	.15541
O	.01240
O-	.00013
OH	.00590
OH-	.00008
O2	.00171

$NANO_3$

AL	.00802
ALH	.00005
ALO	.00268
ALOH	.00069
ALOH+	.07261
ALOH-	.00001
ALO2	.00064
ALO2-	.03285
ALO2H	.00062
AL2O	.00168
AL2O2	.00002
AL2O3(L	.19820
CO	.11243
CO2	.00425
CO2-	.00004
E	.03943
H	.04792
H-	.00004
H2	.01520
H2O	.00449
N	.00004
NO	.00256
NO2-	.00001
N2	.14655
NA	.28619
NA+	.00003
NAH	.00046
NAO	.00106
NAO-	.00004
NAOH	.00166
NA2	.00009
O	.01153
O-	.00014
OH	.00617
OH-	.00010
O2	.00136

KNO_3

AL	.00590
ALH	.00004
ALO	.00194
ALOH	.00069
ALOH+	.06669
ALOH-	.00001
ALO2	.00046
ALO2-	.02871
ALO2H	.00061
AL2O	.00130
AL2O2	.00001
AL2O3(L	.19665
CO	.12363
CO2	.00466
CO2-	.00004
E	.03800
H	.05134
H-	.00004
H2	.02224
H2O	.00649
K	.28177
K+	.00033
KO	.00188
KOH	.00266
K2	.00008
N	.00003
NO	.00213
NO2-	.00001
N2	.14531
O	.00889
O-	.00011
OH	.00641
OH-	.00011
O2	.00134

$CSNO_3$

AL	.00204
ALH	.00003
ALO	.00053
ALOH	.00057
ALOH+	.04328
ALOH-	.00001
ALO2	.00010
ALO2-	.01383
ALO2H	.00043
AL2O	.00038
AL2O3(L	.17604
CO	.18175
CO2	.00582
CO2-	.00005
CS	.25944
CS+	.00093
CSO	.00053
CS2	.00011
E	.03012
H	.05674
H-	.00005
HCO	.00001
H2	.06719
H2O	.01605
N	.00001
NO	.00084
N2	.13572
O	.00261
O-	.00004
OH	.00509
OH-	.00011
O2	.00025

$NACLO_4$

AL	.02525
ALCL	.0311[illegible]
ALCL2	.0013[illegible]
ALH	.00004
ALO	.01123
ALOCL	.00887
ALOH	.00654
ALOH+	.1384[illegible]
ALO2	.[illegible]0345
ALO2-	.[illegible]4245
ALO2H	.000[illegible]
AL2O	.00[illegible]
AL2O2	.0000[illegible]
AL2O3(L	.143[illegible]
CO	.120[illegible]
CO2	.[illegible]0572
CO2-	.0000[illegible]
CL	.[illegible]4477
CL-	.[illegible]659[illegible]
CLO	.0000[illegible]
E	.[illegible]29[illegible]
H	.[illegible]287[illegible]
H-	.00001
HCL	.[illegible]043[illegible]
H2	.[illegible]01[illegible]
H2O	.[illegible]0071
N	.[illegible]00[illegible]
NO	.[illegible]010[illegible]
N2	.[illegible]027[illegible]
NA	.155[illegible]
NA+	.[illegible]000[illegible]
NACL	.[illegible]596[illegible]
NAH	.[illegible]006[illegible]
NAO	.[illegible]01[illegible]
NAO-	.[illegible]000[illegible]
NAOH	.[illegible]0[illegible]3
NA2	.[illegible]0[illegible]
O	.[illegible]495
O-	.[illegible]002[illegible]
OH	.[illegible]054
OH-	.[illegible]00[illegible]
O2	.[illegible]07[illegible]

TABLE 3 (CONT.)

(A) ALUMINUM FUEL (CONT.)

$KClO_4$

AL	.02353
ALCL	.02322
ALCL2	.00077
ALH	.00005
ALO	.01036
ALOCL	.00660
ALOH	.00066
ALOH+	.14229
ALO2	.00315
ALO2-	.04769
ALO2H	.00073
AL2O	.00629
AL2O2	.00007
AL2O3(L)	.14068
CO	.13098
CO2	.00616
CO2-	.00003
CL	.03367
CL-	.06037
CLO	.00002
E	.03444
H	.03582
H-	.00002
HCL	.00428
H2	.00304
H2O	.00115
K	.12676
K+	.00061
KCL	.09005
KO	.00186
KOH	.00045
K2	.00031
N	.00002
NO	.00161
N2	.00307
O	.04638
O-	.00028
OH	.00670
OH-	.00005
O2	.00695

NaO_2

AL	.01043
ALH	.00005
ALO	.00371
ALOH	.00070
ALOH+	.08062
ALOH-	.00001
ALO2	.00094
ALO2-	.03894
ALO2H	.00066
AL2O	.00252
AL2O2	.00002
AL2O3(L)	.18772
CO	.10940
CO2	.00434
CO2-	.00004
E	.04132
H	.04572
H-	.00003
H2	.01083
H2O	.00339
N	.00001
NO	.00044
N2	.00274
NA	.42585
NA+	.00005
NAH	.00057
NAO	.00187
NAO-	.00006
NAOH	.00211
NA2	.00019
O	.01631
O-	.00017
OH	.00643
OH-	.00009
O2	.00200

Na_2O_2

AL	.00002
ALOH	.00001
ALOH+	.00067
AL2O3(S)	.14299
CO	.10460
CO2	.00010
E	.00067
H	.00191
H2	.07339
H2O	.00037
N2	.00273
NA	.62854
NAH	.00161
NAOH	.00051
NA2	.00167

H_2O_2

AL	.01214
ALH	.00022
ALO	.00451
ALOH	.00311
ALOH+	.18339
ALOH-	.00006
ALO2	.00118
ALO2-	.09079
ALO2H	.00302
AL2O	.00296
AL2O2	.00003
AL2O3(L)	.12690
E	.09091
H	.19859
H-	.00029
H2	.17269
H2O	.05619
O	.01990
O-	.00042
OH	.02937
OH-	.00082
O2	.00258

$-CF_2-$

ALF	.0377
ALF2	[illegible]
ALF3	[illegible]
C(S)	.44560
C	[illegible]
CF	.02399
CF2	.00529
CF3	[illegible]
CF4	.00071
CN	.00027
C2	.00046
C2F2	.00002
C2N	.00317
C2N2	.00035
C3	[illegible]
C4	.00002
C5	.00013
F	.07765
FCN	.00135
N	[illegible]
N2	.11478

AIR

AL	.03271
AL+	.00013
ALO	.01442
ALO2	.00230
ALO2-	.00007
AL2O	.00991
AL2O2	.00004
AL2O3(L)	.13498
E	.00006
N	.00023
NO	.01087
N2	.79492
O	.03002
O2	.00329

O_2

AL	.17857
AL+	.00139
ALO	.10052
ALO2	.03717
ALO2-	.00105
AL2O	.06625
AL2O+	.00004
AL2O2	.00093
AL2O3(L)	.21118
E	.00037
O	.34016
O-	.00001
O2	.06237

TABLE 3 (CONT.)
(B) MAGNESIUM FUEL

$LINO_3$

CO	.06558
CO2	.01967
E	.00015
H	.01087
H2	.00468
H2O	.01032
LI	.13264
LI+	.00015
LIH	.00034
LIO	.00716
LIOH	.06721
LI2	.00007
LI2O	.00008
LI2O2	.00005
MG	.08097
MGH	.00017
MGN	.00001
MGO(S)	.37868
MGO	.05814
MGOH	.00650
MGO2H2	.00012
N	.00001
NO	.00469
N2	.11183
O	.01221
OH	.00861
O2	.01087

$NANO_3$

CO	.06986
CO2	.01981
E	.00027
H	.01753
H2	.01266
H2O	.02634
MG	.08254
MGH	.00029
MGN	.00001
MGO(S)	.36403
MGO	.05507
MGOH	.01031
MGO2H2	.00030
N	.00001
NO	.00406
N2	.10146
NA	.18902
NA+	.00028
NAH	.00029
NAO	.00223
NAOH	.01035
NA2	.00007
O	.01098
OH	.01299
O2	.00922

KNO_3

CO	.07747
CO2	.02140
CO2-	.00001
E	.00115
H	.01791
H2	.01455
H2O	.02936
K	.18378
K+	.00119
KO	.00446
KOH	.01412
K2	.00005
MG	.07728
MGH	.00029
MGN	.00001
MGO(S)	.36118
MGO	.04886
MGOH	.01028
MGO2H2	.00031
N	.00001
NO	.00368
NO2-	.00001
N2	.10255
O	.00956
O-	.00001
OH	.01270
OH-	.00002
O2	.00779

$CSNO_3$

CO	.11977
CO2	.02735
CO2-	.00003
CS	.19226
CS+	.00257
CSO	.00156
CS2	.0000[illegible]
CS2O	.00001
E	.00247
H	.02163
H2	.03227
H2O	.05265
MG	.05958
MGH	.00031
MGN	.00001
MGO(S)	.32891
MGO	.02699
MGOH	.01060
MGO2H2	.00042
NO	.00205
NO2-	.00001
N2	.10169
O	.00454
O-	.00001
OH	.01128
OH-	.00004
O2	.00391

$NACLO_4$

CO	.07697
CO2	.02604
CL	.02031
CL-	.00063
CLO	.00003
E	.00007
H	.02119
HCL	.01502
H2	.01067
H2O	.02702
MG	.11067
MGCL	.01064
MGCL2	.01151
MGH	.00035
MGO(L)	.31625
MGO	.10027
MGOH	.01323
MGO2H2	.00037
NO	.00107
N2	.00215
NA	.06325
NA+	.00070
NACL	.09784
NAH	.00009
NAO	.00115
NAOH	.00345
NA2	.00001
NA2CL2	.00001
O	.02439
OH	.02030
O2	.02483

$KCLO_4$

CO	.08410
CO2	.02680
CL	.01458
CL-	.00183
CLO	.00002
F	.00028
H	.02308
HCL	.01189
H2	.01282
H2O	.03055
K	.04183
K+	.00213
KCL	.11808
KO	.00154
KOH	.00312
MG	.11648
MGCL	.00810
MGCL2	.00609
MGH	.00040
MGO(L)	.31394
MGO	.09898
MGOH	.01440
MGO2H2	.00042
NO	.00104
N2	.00237
O	.02263
OH	.02077
OH-	.00001
O2	.02170

NAO_2

CO	.06852
CO2	.01978
E	.00036
H	.01758
H2	.01133
H2O	.02408
MG	.09070
MGH	.00030
MGO(S)	.35046
MGO	.06323
MGOH	.01059
MGO2H2	.00029
NO	.00063
N2	.00199
NA	.28385
NA+	.00037
NAH	.00041
NAO	.00359
NAOH	.01464
NA2	.00015
O	.01275
OH	.01348
OH-	.00001
[illegible]	.01093

NA_2O_2

CO	.082[illegible]6
CO2	.001[illegible]2
E	.00001
H	.00212
H2	.05296
H2O	.00370
MG	.00797
MGH	.00004
MGO(S)	.38600
MGO	.00005
MGOH	.00029
N2	.00218
NA	.45443
NA+	.00001
NAH	.00118
NAO	.00001
NAOH	.00442
NA2	.00112
OH	.00003

H_2O_2

E	.00001
H	.06312
HO2	.00001
H2	.09400
H2O	.18593
MG	.14356
MG+	.00001
MGH	.00131
MGO(L)	.28792
MGO	.10086
MGOH	.03932
MGO2H2	.00255
O	.01913
OH	.04705
O2	.01522

$-CF_2-$

C(S)	.453[illegible]
C	.0[illegible]
CF	[illegible]
CF2	[illegible]
CN	[illegible]
C2	[illegible]
C2N	[illegible]
C2N2	[illegible]
C3	[illegible]
C4	[illegible]
C5	[illegible]
F	.[illegible]3[illegible]
FCN	[illegible]
MG	[illegible]
MGF	[illegible]
MGF2	.44[illegible]
N	[illegible]
N2	[illegible]

AIR

MG	.10593
MGN	.00003
MGO(S)	.20054
MGO	.06007
N	.00001
NO	.00892
N2	.60611
O	.01060
O2	.00778

O_2

E	.00002
MG	.23629
MG+	.000[illegible]
MGO(L)	.32379
MGO	.28228
O	.07658
O2	.08109

TABLE 3 (CONT.)

(C) BERYLLIUM FUEL

$NANO_3$

BE	.02246
BEH	.00012
BEN	.00001
BEO(L)	.48916
BEO	.00284
BEOH	.00406
BEO2H2	.00028
BE2O	.00538
BE2O2	.00333
BE3O3	.00404
BE4O4	.00146
CO	.06565
CO2	.00172
E	.00113
H	.05440
H2	.01322
H2O	.00279
N	.00006
NO	.00228
N2	.10226
NA	.20007
NA+	.00114
NAH	.00038
NAO	.00080
NAOH	.00084
NA2	.00006
O	.01335
OH	.00556
O2	.00112

$NACLO_4$

BE	.04991
BECL	.01479
BECL2	.01031
BEH	.00019
BEO(L)	.42969
BEO	.00852
BEOH	.00589
BEO2H2	.00023
BE2O	.01375
BE2O2	.00919
BE3O3	.00870
BE4O4	.00303
CO	.07363
CO2	.00235
CL	.06224
CL-	.00197
CLO	.00004
CL2	.00001
E	.00073
H	.06391
HCL	.01122
H2	.00763
H2O	.00201
N	.00002
NO	.00067
N2	.00163
NA	.10686
NA+	.00271
NACL	.04994
NAH	.00015
NAO	.00078
NAOH	.00035
NA2	.00001
O	.04338
O-	.00001
OH	.00899
O2	.00452

$-CF_2-$

BE	.00047
BEF	.05564
BEF2	.47359
C(S)	.41065
C	.00386
CF	.00842
CF2	.00022
C2	.00367
C3	.02649
C4	.00017
C5	.00038
F	.01944

AIR

BE	.03130
BEN	.00044
BEO(L)	.25344
BEO	.00378
BE2O	.00739
BE2O2	.00447
BE3O3	.00555
BE4O4	.00282
N	.00019
NO	.00644
N2	.66693
O	.01749
O2	.00140

(D) BORON FUEL

$NACLO_4$

BCL	.00003
BO	.09121
BOCL	.00985
BO2	.08641
BO2-	.00298
B2O2	.00243
B2O3	.18113
CO	.11132
CO2	.01329
CL	.04595
CL-	.00037
CLO	.00003
CL2	.00001
E	.00003
H	.12536
HBO	.00009
HBO2	.07638
HCL	.02866
H2	.01078
H2O	.00951
NO	.00052
N2	.00299
NA	.07967
NA+	.00337
NACL	.19668
NAH	.00004
NAO	.00050
NAOH	.00128
NA2	.00001
NA2CL2	.00003
O	.01214
OH	.00853
O2	.00436

$NANO_3$

B	.00331
BO2	.00017
BO2-	.00014
B2O2	.00494
B2O3(L)	.05637
B2O3	.213[illegible]2
CO	.16619
CO2	.00081
H	.00088
HBO	.00003
HBO2	.05768
H2	.04542
H2O	.00174
N2	.17242
NA	.33551
NA+	.00014
NAH	.00008
NAOH	.00187
NA2	.00057

$-CF_2-$

H	.00001
BF	.03414
BF2	.05200
BF3	.31903
C(S)	.52379
C	.00172
CF	.01594
CF2	.00172
C2	.00149
C3	.01133
C4	.00006
C5	.00014
F	.04160

AIR

B(L)	.02097
B	.00113
BN(S)	.26109
BN	.00019
BO	.13511
BO2	.00064
B2O	.00082
B2O2	.07546
B2O3	.00272
N2	.49461

TABLE 3 (CONT.)

(E) IRON FUEL

$NANO_3$		$NACLO_4$	
CO	.00035	CO	.06781
CO2	.19664	CO2	.09023
FE3O4(S)	.16284	CL	.00582
H2	.00001	CLO	.00001
H2O	.01077	FE	.00356
NO	.00036	FECL	.00011
N2	.22854	FECL2	.00269
NA	.07983	FEO(L)	.47530
NAO	.00135	FEO	.00233
NAOH	.26280	FEO2H2	.00034
NA2	.00018	H	.00445
NA2O(L)	.05049	HCL	.01829
NA2O2H2	.00099	H2	.00970
O	.00001	H2O	.08551
OH	.00007	NO	.00555
O2	.00564	N2	.00384
		NA	.02388
		NACL	.17555
		NAH	.00003
		NAO	.00039
		NAOH	.00531
		NA2CL2	.00014
		O	.00365
		OH	.01029
		O2	.01163

(F) SILICON FUEL

$NANO_3$		$NACLO_4$		AIR	
CO	.05881	CO	.06509	NO	.01191
CO2	.04700	CO2	.05618	N2	.75496
E	.00014	CL	.02827	O	.00835
H	.00741	CL-	.00056	O2	.01863
H2	.00766	CLO	.00007	SIO	.10133
H2O	.04237	CL2	.00001	SIO2(L)	.09933
NO	.00505	E	.00003	SIO2	.00546
NO2-	.00001	H	.01255		
N2	.14794	HCL	.02444		
NA	.25677	HO2	.00001		
NA+	.00016	H2	.00746		
NAH	.00027	H2O	.04639		
NAO	.00408	NO	.00155		
NAOH	.03386	N2	.00239		
NA2	.00614	NA	.04607		
O	.00741	NA+	.00059		
OH	.01223	NACL	.18315		
O2	.01671	NAH	.00005		
SIO	.08778	NAO	.00130		
SIO2(L)	.25936	NAOH	.00535		
SIO2	.00484	NA2CL2	.00004		
		O	.02715		
		OH	.02622		
		O2	.06834		
		SIO	.24496		
		SIO2(L)	.13462		
		SIO2	.01713		

(G) CARBON FUEL

$NANO_3$		$NACLO_4$		AIR	
CO	.00037	CO	.23958	CO	.02530
CO2	.48580	CO2	.34170	CO2	.17610
H2O	.00164	CL	.01412	NO	.00166
NO	.00011	CL-	.00025	N2	.79398
N2	.20814	CLO	.00002	O	.00018
NA	.02491	CL2	.00001	O2	.00278
NAO	.00024	E	.00001		
NAOH	.16936	H	.00523		
NA2	.00001	HCL	.02177		
NA2O(L)	.10782	H2	.00564		
OH	.00001	H2O	.05393		
O2	.00157	NO	.00080		
		N2	.00257		
		NA	.02970		
		NA+	.00026		
		NACL	.22502		
		NAH	.00002		
		NAO	.00058		
		NAOH	.00561		
		NA2CL2	.00011		
		O	.00802		
		OH	.01363		
		O2	.03143		

THERMITE @ 3017K

AL	.00047
ALO	.00008
AL2O	.00007
AL2O3(L)	.31295
FE(L)	.54631
FE	.07952
FEO	.00075
NO	.00005
N2	.05471
O	.00007

TABLE 4

Computed Densities (g/cc) of Fuel-Oxidizer Combinations.

	$LiNO_3$	$NaNO_3$	KNO_3	$CsNO_3$	$KClO_4$	Na_2O_2	H_2O_2	$-CF_2-$
Al	2.28	2.20	2.09	3.00	2.34	2.49	1.88	2.32
Mg	1.91	1.88	1.84	2.65	2.01	2.13	1.59	2.02
Be		1.97						2.11
B		2.11						2.23
Fe		2.81						
Si		2.12						
C		2.09						

TABLE 5

Computed adiabatic temperatures for the combustion of aluminum compounds.

	Reaction	Temperature (K)
	$2Al + NaNO_3$	3758
	$Al_4C_3 + 3\ NaNO_3$	3321
	$3\ Mg + NaNO_3$	3158
	$6\ Mg_4Al_3 + 17\ NaNO_3$	3147
*	$AlH_3 + NaNO_3$	2879
*	$3\ MgAl_2H_8 + 8\ NaNO_3$	2794
*	$6\ LiAlH_4 + 7\ NaNO_3$	2448
	$Al_2S_3 + 3\ NaNO_3$	1616

* A considerably higher adiabatic temperature would probably be computed for a more fuel-rich mixture.

TABLE 6

Computed adiabatic temperature for enrichment with sodium compounds.

Fuel Compound Added	Temperature (K)
No additive	3158
Na	3098
Na_2C_2	3048
NaH	3046
Na_2S	3017
NaN_3	3010
$NaNH_2$	2987